Planar Boron Clusters

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An interesting feature of elemental boron and boron compounds is the occurrence of highly symmetric icosahedral clusters. The rich chemistry of boron is also dominated by three-dimensional cage structures. Despite its proximity to carbon, elemental boron clusters have been scarcely studied experimentally and their structures and chemical bonding have not been fully elucidated. Our combined experimental and theoretical studies have shown that small boron clusters all prefer planar structures and exhibit aromaticity and antiaromaticity according to the Hückel rules, akin to planar hydrocarbons. Aromatic boron clusters possess more circular shapes whereas antiaromatic boron clusters are elongated, analogous to structural distortions of antiaromatic hydrocarbons. The planar boron clusters are thus the only series of molecules other than the hydrocarbons to exhibit size-dependent aromatic and antiaromatic behavior and represent a new dimension of boron chemistry. The stable aromatic boron clusters may exhibit similar chemistries as that of benzene, such as forming sandwich-type metal compounds. These studies have been featured in Chem. & Eng. News (March 1, 2004). [H. J. Zhai, K. Kiran, J. Li, and L. S. Wang, Nature Materials 2, 827-833 (2003)]

